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Impact on Model Uncertainty of Diabatization in Distillation Columns

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1. Introduction

Studies show that operating a Conventional Distillation Column (CDiC) with internal heat transfer (diabatically) can reduce cost of separation. An example is the Heat-Integrated Distillation Column (HIDiC) illustrated in Figure 1.

The majority of studies of the HIDiC are concerned with the potential energy savings and operability, and only a limited amount of model validations have been carried out due to scarcity of experimental data.

The purpose of this study is to perform uncertainty and sensitivity analysis on steady state simulations on conventional and heat-integrated distillation columns.

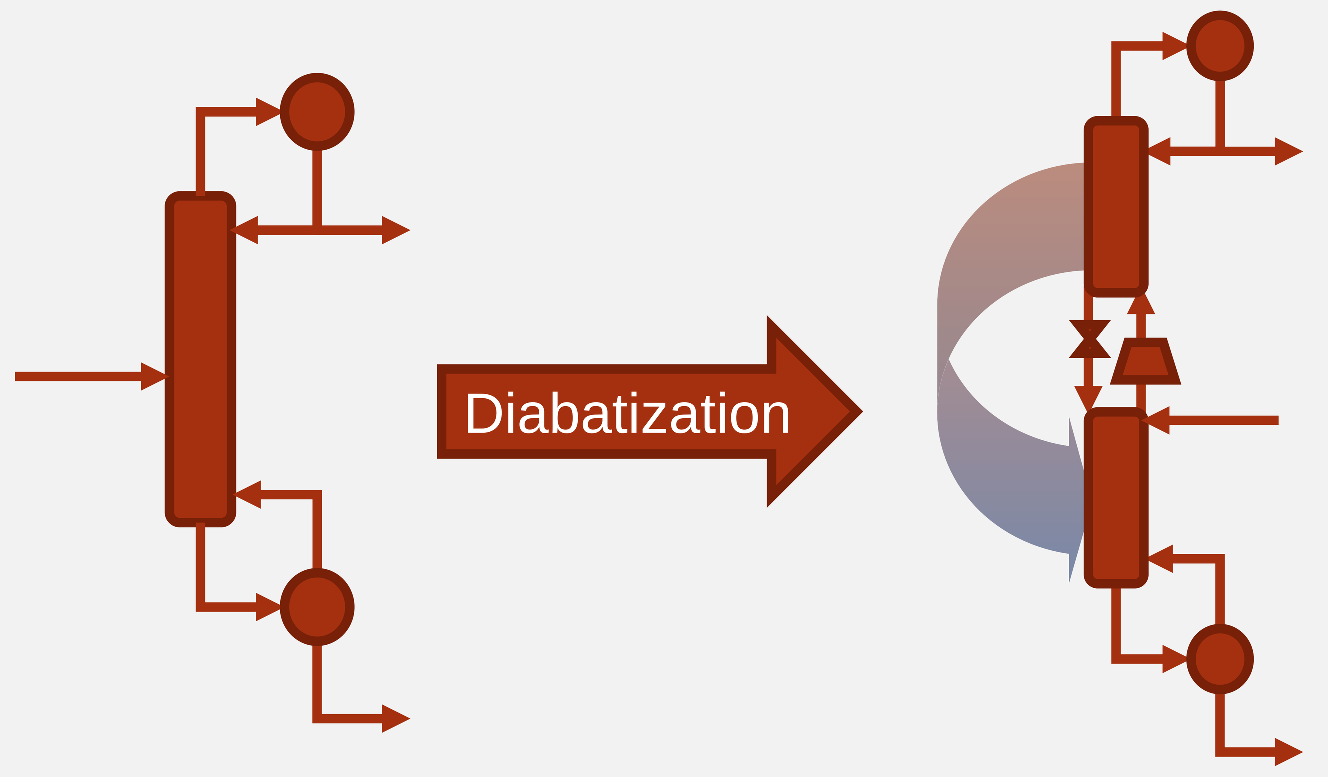

Figure 1. Diabatization of a CDiC (left) to obtain a HIDiC (right).

2. Methods

This study considers 12 separations:

- Benzene/Toluene (BT) and Benzene/Flourobenzene (BF)
- Low purity (95% / 5%) and high purity (99% / 1%)
- CDiC, HIDiC and iHIDiC (with only feed preheater)

Classification:

- Variables: $\boldsymbol{u} = (P_r, P_s, q, L_C, V_R, F, z)^T$
- Parameters: $\boldsymbol{\theta} = (\alpha, \lambda, A_{Ant}, B_{Ant}, C_{Ant}, U, A, M, T_\sigma, \gamma, \eta_c, S_{water}, S_{steam}, S_{electricity}, T_{water}, T_{steam})^T$
- Output: $\boldsymbol{y} = (\eta_{2nd}, OPEX, CAPEX, \tau_1)^T$

Distributions of selected uncertain parameters:

Heat of vaporization:	$\lambda \sim \mathcal{N}(\lambda_0, 0.975^2\lambda_0^2)$
Relative volatility:	$\alpha \sim \mathcal{U}(0.99\alpha_0, 1.01\alpha_0)$
Heat transfer coefficient:	$UA \sim \mathcal{U}(0.90UA_0, 1.10UA_0)$
Stage holdup:	$M \sim \mathcal{U}(0.95M_0, 1.05M_0)$
Adiabatic index:	$\gamma \sim \mathcal{U}(0.95\gamma_0, 1.05\gamma_0)$

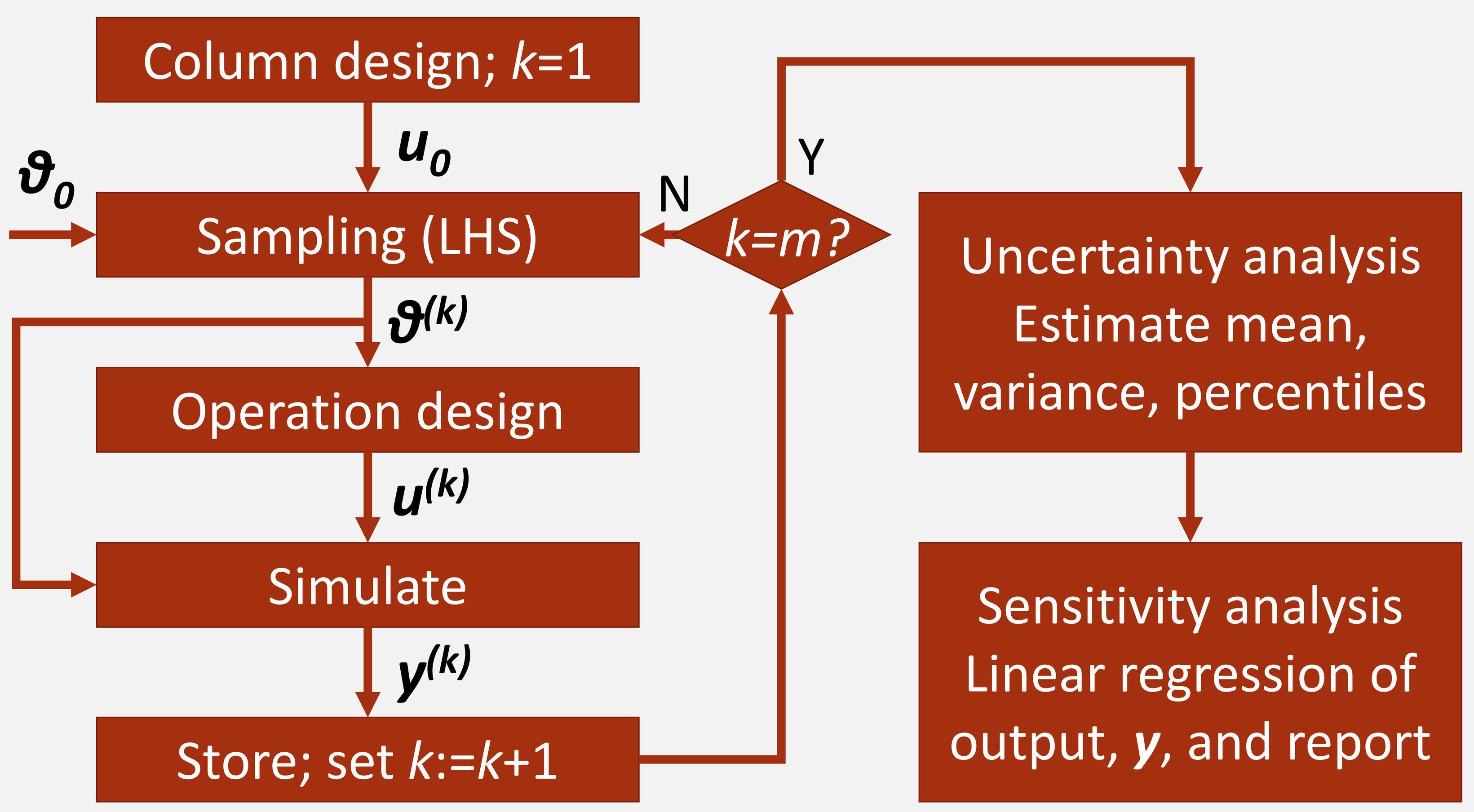

Figure 2. Applied algorithm.

3. Results

Uncertainty analysis

- **Q:** How does the HIDiC perform compared the CDiC, and (if) is the improvement significant? **A:** Table 1 and Figure 3.

Table 1. Nominal operating conditions.

ID	Config.	Mixture	X	α	N_S	A, m²	q	P_r/P_s	L_C/D	V_R/B
A1	CDiC	BT	0.95	2.4	20	0	1	1	1.26	2.26
B1	HIDiC	BT	0.95	2.4	20	2.5	1	2.93	0.27	1.27
C1	iHIDiC	BT	0.95	2.4	20	5.0	0.5	2.93	0	0
A2	CDiC	BT	0.99	2.4	30	0	1	1	1.44	2.44
B2	HIDiC	BT	0.99	2.4	30	2.5	1	2.89	0.28	1.28
C2	iHIDiC	BT	0.99	2.4	30	5.0	0.5	2.89	0	0
A3	CDiC	BF	0.95	1.2	76	0	1	1	10.0	11.0
B3	HIDiC	BF	0.95	1.2	76	7.5	1	1.70	4.17	5.17
C3	iHIDiC	BF	0.95	1.2	76	15	0.5	1.70	0	0
A4	CDiC	BF	0.99	1.2	118	0	1	1	10.7	11.7
B4	HIDiC	BF	0.99	1.2	118	7.5	1	1.55	4.29	5.29
C4	iHIDiC	BF	0.99	1.2	118	15	0.5	1.55	0	0

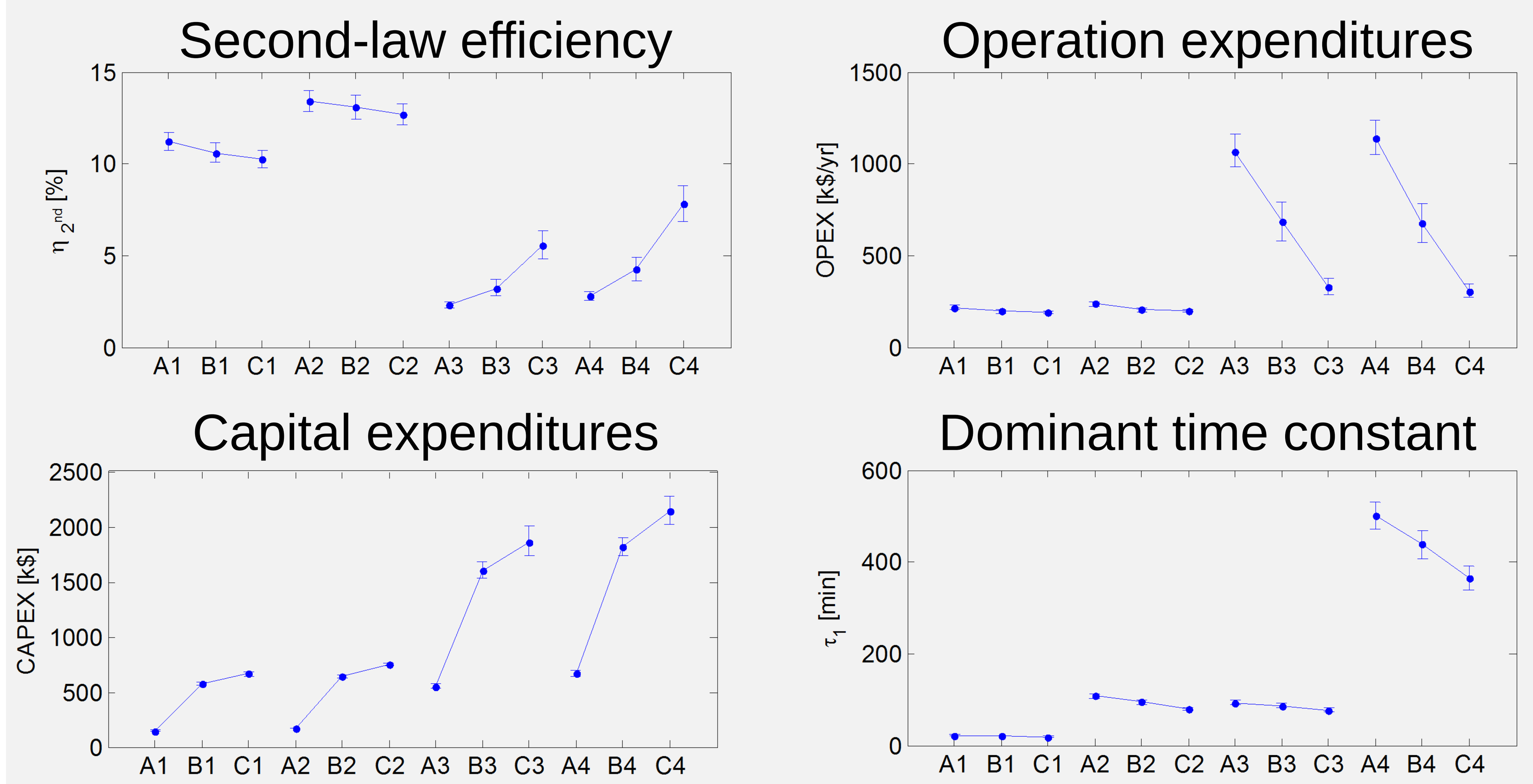

Figure 3. Performance indicators with 95% confidence intervals.

Sensitivity Analysis

- **Q:** Which uncertain parameters have the most significant contribution on uncertainty? **A:** Figure 4.

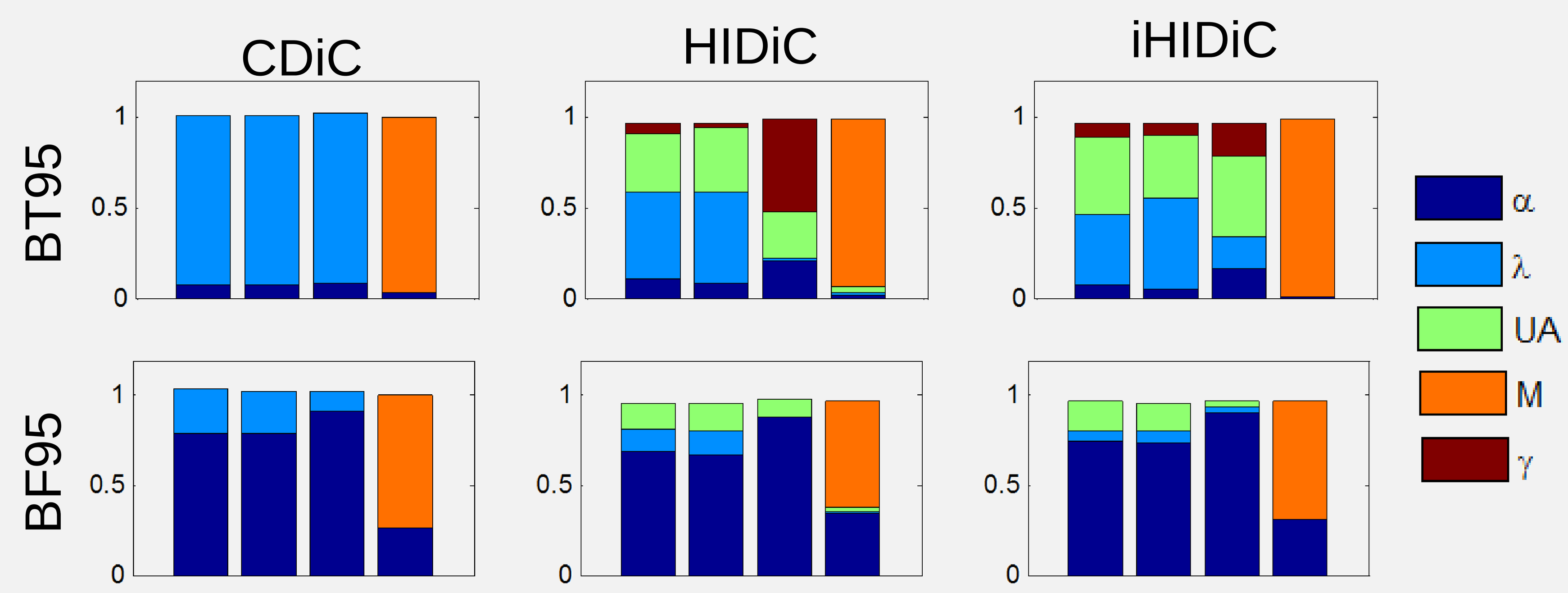

Figure 4. Squared linear regression parameters. Impact on uncertainty is related to the magnitude of individual contributions.

4. Conclusions

- Calculations related to compressor are uncertain (e.g. duty)
- Linear correlation for HIDiC between α and η_{2nd} and *OPEX*, *CAPEX* and τ_1
- Significant uncertainty in η_{2nd} and *OPEX* for HIDiC with many stages
- U has significance on variance in η_{2nd} and *OPEX*, *CAPEX* and τ_1 for HIDiC with fewer stages